Wick theorem

Motivation for the Wick theorem. The Wick theorem is an essential tool for performing calculations in any field theory. It allows us to represent the expectation value of a product of many operators (that is hard to calculate) as a sum of terms that involve only products of two operators (that are less hard to calculate). Below you will prove the Wick theorem.

Exercise 1: Proof of the Wick theorem (4 points): Let us start with the formal expression of the Wick decomposition:

$$\langle AB \ldots YZ \rangle = \contraction{}{A}{}{B}AB \ldots \contraction{}{Y}{}{Z}YZ + \contraction{}{A}{B\ldots}{Y}\contraction[2ex]{A}{B}{\ldots Y}{Z}AB \ldots YZ + \ldots, \tag{1}$$

where the sum on the right-hand side runs over all complete contractions, i.e., over all the contractions that have every operator contracted. The definition of the contraction is

$$\contraction{}{A}{}{B}AB = \langle AB \rangle. \tag{2}$$

To summarize, the Wick decomposition is an expression of the many-operator average as a sum of the products of two-operator averages, or in the language of Green functions, an expansion of many-particle Green function into a sum of products of single-particle Green functions.

The **Wick theorem** states that any theory described by a density matrix of the form $\rho = \mathrm{e}^{\mathcal{A}}$, with $\mathcal{A}$ a 1-particle operator admits a Wick decomposition. Such an $\mathcal{A}$ can be written as

$$\mathcal{A} = \sum_a A_a a_a^\dagger a_a, \tag{3}$$

where $a_a^\dagger, a_a$ are either boson or fermion operators (depending on the underlying theory).

(a) Show that the equation of motion for each operator $\rho = \rho(t_0)$, $A = A(t_1)$, $B = B(t_2)$, $\ldots$, $Y = Y(t_{n-1})$, $Z = Z(t_n)$ is identical on the left- and on the right-hand side of (1).

Due to this it is sufficient to prove (1) for the case when all the operators have the same time argument t_0: $\rho = \rho(t_0)$, $A = A(t_0)$, $\ldots$, $Y = Y(t_0)$, $Z = Z(t_0)$. This allows us to use the (anti)commutation relations between the operators, because these are *only valid between operators with equal time arguments* (never forget that!!!).

(b) Working in the occupation number basis

$$|\{n_a\}\rangle = |n_1, n_2, \ldots\rangle = \left(\prod_a \frac{(a_a^\dagger)^{n_a}}{\sqrt{n_a!}} \right) |0\rangle, \tag{4}$$

show that we can write

$$\tag{5}$$

$$\rho = \sum_{\{n_a\}} |\{n_a\}\rangle \mathrm{e}^{\sum_a A_a n_a} \langle \{n_a\}|, \tag{6}$$

with $n_a = a_a^\dagger a_a$.

(c) Let α_a denote either a creation or an annihilation operator, $\alpha_a \in \{a_a^\dagger, a_a\}$. Show that $\alpha_a \rho = \zeta_a \rho \alpha_a$, where $\zeta_a = \mathrm{e}^{A_a}$ if $\alpha_a = a_a$, and $\zeta_a = \mathrm{e}^{-A_a}$ if $\alpha_a = a_a^\dagger$.

(d) Prove that

$$\begin{aligned} \mathrm{Tr}\left(\rho \alpha_a \alpha_b \ldots \alpha_y \alpha_z\right) &= \frac{[\alpha_a, \alpha_b]_\pm}{1 \pm \zeta_a} \mathrm{Tr}\left(\rho \alpha_c \alpha_d \ldots \alpha_y \alpha_z\right) \\ &\mp \frac{[\alpha_a, \alpha_c]_\pm}{1 \pm \zeta_a} \mathrm{Tr}\left(\rho \alpha_b \alpha_d \ldots \alpha_y \alpha_z\right) + \ldots \\ &+ \frac{[\alpha_a, \alpha_z]_\pm}{1 \pm \zeta_a} \mathrm{Tr}\left(\rho \alpha_b \alpha_c \ldots \alpha_y\right), \end{aligned} \tag{7}$$

where the + sign in the last line of (7) corresponds to an even number of α operators in the trace. *Hint*: commute the α_a operator to the right end of the expression under the trace, then use the cyclic property of the trace to move α_a back to the left end of the expression, and apply (c).

(e) Show that

$$\overline{\alpha_a\alpha_b} = \mathrm{Tr}\,(\rho\alpha_a\alpha_b) = \frac{[\alpha_a, \alpha_b]_\pm}{1 \pm \zeta_a}. \tag{8}$$

(f) Use (d) and (e) to prove that the Wick decomposition holds in a theory described by the density matrix $\rho = \mathrm{e}^{\mathcal{A}}$, assuming that $A = \alpha_a, B = \alpha_b, \ldots, Z = \alpha_z$.

Exercise 2 (4 points) Further inquiries.

(a) Assume now that we have exotic quasi-particles that mix fermion and boson properties such that $\{a_a\,,\, a_b^\dagger\} = \mathrm{e}^{i\phi}\delta_{ab}, \{a_a\,,\, a_b\} = 0$ for some given phase ϕ (such collective modes can be found, for instance, in fractional quantum Hall systems). Does a Wick theorem still hold? What would be the modification?

(b) What about a Wick theorem for spin operators? The latter do not obey regular commutation or anticommutation rules, but obey the algebra $\left[S_a^\alpha\,,\, S_b^\beta\right] = i\hbar \sum_\gamma \epsilon^{\alpha\beta\gamma} S_a^\gamma \delta_{ab}$, with a, b labeling, say, different lattice sites, $\alpha, \beta, \gamma \in \{x, y, z\}$, and $\epsilon^{\alpha\beta\gamma}$ the Levi-Civita symbol (the fully antisymmetric tensor).

(c) What happens if we have a system described by $H = H_0^f + H_0^b$, with H_0^f quadratic in fermion operators f_a and H_0^b quadratic in boson operators b_a? Use the example of $\langle f_a^\dagger b_b f_c b_d^\dagger\rangle$ for your argument.

(d) Beware the following trap: Assume that $A = a_a^\dagger a_b, B = a_c^\dagger, C = a_d$, and $D = a_e^\dagger a_f$. We then have $\overline{AB} = \overline{AC} = \overline{BD} = \overline{CD} = 0$ because particle numbers are not conserved in the averages. Therefore the application of the Wick theorem reduces to $\langle ABCD\rangle = \overline{A\,\overline{BC}\,D}$. Show that this is *wrong* and explain in 2 words (or so...) what needs to be done to avoid such errors. Compare with Exercise 1, (f).

Exercise 3 (2 points) Application of the Wick theorem.

(a) Consider the time ordered (real time or contour time) 2-particle Green's function

$$\chi^c(r) = -i\langle T\{\psi^\dagger(r)\psi(r)\psi^\dagger(0)\psi(0)\}\rangle_0, \tag{9}$$

where $r = (\mathbf{x}, t)$, the $\psi(r)$ are fermion field operators, and the time evolution is determined by a Hamiltonian H_0 that is quadratic in ψ and $\psi^\dagger$ (such that the Wick theorem can be used).

Show that χ^c decomposes into

$$i\chi^c(r) = \bar{\rho}(r)\bar{\rho}(0) + G^c(r)G^c(-r), \tag{10}$$

with $\bar{\rho}(r) = \langle\psi^\dagger(r)\psi(r)\rangle = -iG^c(x = 0, t = 0^+)$ and $G^c(r)$ as defined in the lectures.

(b) Consider now the retarded 2-particle Green's function

$$\chi^r(r) = -i\theta(t)\langle\left[\psi^\dagger(r)\psi(r)\,,\, \psi^\dagger(0)\psi(0)\right]\rangle_0, \tag{11}$$

and show that

$$i\chi^r(r) = G^r(r)G^<(-r) + G^<(r)G^a(-r), \tag{12}$$

with again the Green's functions as defined in the lectures.

Note that this is a very different result as in Eq. (10): The bare averages $\bar{\rho}$ cancel out with the commutator, while the product G^cG^c is replaced by the sum $G^rG^< + G^<G^a$. This example shows that splitting a many-particle Green's function into single-particle Green's functions works best for time-ordered functions, while retarded, advanced, ... Green's functions always involve more terms and mix the various types of Green's functions.